

On the free volume in nuclear multifragmentation

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In many statistical multifragmentation models the volume available to the N nonoverlapping fragments forming a given partition is a basic ingredient serving to the simplification of the density of states formula. One therefore needs accurate techniques for calculating this quantity. While the direct Monte-Carlo procedure consisting of randomly generating the fragments into the freeze-out volume and counting the events with no overlapped fragments is numerically affordable only for partitions with small N , the present paper proposes a Metropolis - type simulation which allows accurate evaluations of the free volume even for cases with large N . This procedure is used for calculating the available volume for various situations. Though globally this quantity has an exponential dependence on N , variations of orders of magnitude for partitions with the same N may be identified. A parametrization based on the virial approximation adjusted with a calibration function, describing very well the variations of the free volume for different partitions having the same N is proposed. This parametrization was successfully tested within the microcanonical multifragmentation model from [Al. H. Raduta and Ad. R. Raduta, Phys. Rev. C **55**, 1344 (1997); *ibid.*, **56**, 2059 (1997)]. Finally, it is proven that parametrizations of the free volume solely dependent on N are rather inadequate for multifragmentation studies producing important deviations from the exact results.

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I. INTRODUCTION

Nuclear multifragmentation is intensely studied both theoretically and experimentally from more than fifteen years. Since it concerns the decay of excited systems formed in violent heavy ion collisions supposed to be statistically equilibrated, this process has often been described by means of statistical models (e.g. [1–4]). A basic ingredient of some of these models is the volume disponible to N nonoverlapping fragments (often called free volume and denoted herein by Ω_{eff}), positioned into a freeze-out volume Ω . This serves to the simplification of the density of states formula and implicitly to an easier evaluation of the various statistical observables. For the case of N noninteracting particles, Ω_{eff} is simply given by Ω^N . When the fragments are not allowed to overlap each other - which is the physical case, this quantity is drastically limited. In statistical models Ω_{eff} manifests as a factor entering the statistical weights of the fragment partitions and thus the accuracy of the model predictions is directly influenced by the quality of the Ω_{eff} parametrization. While an exact analytical evaluation of the N -dimensional integral defining Ω_{eff} is up to now practically impossible, various approximations for this quantity have been reported

since the beginning of the multifragmentation studies [4,5,1].

The topic of the effective volume goes far beyond the nuclear fragmentation studies being a fundamental thermodynamical problem. Fields like chemical physics, solid state physics and others are dealing with such problems. Here it is worth mentioning the approaches corresponding to infinite systems composed of identical or non identical spherical fragments proposed more then thirty years ago [6,7]. While the above approaches are accurate for the systems they have been designed for, from the point of view of the nuclear multifragmentation studies they have two important drawbacks: they do not account for the *finite* volume of the freeze-out recipient in which fragmentation is supposed to take place and they have complicated expressions making them unsuitable to be employed in a time consuming Metropolis sharp microcanonical multifragmentation calculation.

So far, accurate predictions of Ω_{eff} have been performed via a simple Monte Carlo method consisting of randomly generating the fragments into the freeze-out volume and counting the events in which no two fragments are overlapped [8,9]. However, though it provides exact evaluations of Ω_{eff} (within the statistical error), this method is numerically affordable only for cases with small number of fragments. Indeed, since Ω_{eff} is exponentially decreasing with N , accurate evaluations for large N are possible only with prohibitively large numbers of events.

The present paper proposes a Metropolis-type simulation procedure which makes possible exact evaluations of Ω_{eff} even for partitions with large number of fragments. Since variations of χ (defined as Ω_{eff}/Ω^N) of orders of magnitude are observed for partitions with the same N but different fragments size distribution a parametrization of χ only dependent of N appears to be inadequate. For this reason a parametrization based on an adjusted virial approximation is proposed.

The paper is organized as follows: Section II gives a description of the standard Monte Carlo method and proposes a Metropolis type procedure allowing exact calculations of χ even for large N . Section III presents a brief overall view on the results of the proposed method. In Section IV, a virial parametrization of χ is proposed. Applications and tests of the resulted parametrizations within the microcanonical multifragmentation model [10,11] are presented in Section V. The conclusions are drawn in Section VI.

II. CALCULATING PROCEDURE

Suppose that we are dealing with N spherical fragments of sizes A_i , $i = 1, \dots, N$ resulted from a spherical source nucleus of size A : $\sum_{i=1}^N A_i = A$, positioned at \mathbf{r}_i , $i = 1, \dots, N$ into a freeze-out recipient having the volume $\Omega = n \Omega_0$, where Ω_0 is the volume of the source nucleus at normal nuclear matter density: $\Omega_0 = 4\pi r_0^3 A/3$, $r_0 = 1.2$ fm. The fragments are not allowed to overlap one another or the recipient “walls” meaning that they are subject to the constrains: $\prod_{i<j}^N \theta_{ij} \prod_{i=1}^N \theta_i^r$ with $\theta_{ij} = \Theta(|\mathbf{r}_i - \mathbf{r}_j| - (R_i + R_j))$, $\theta_i^r = \Theta(R - R_i - |\mathbf{r}_i|)$, where $R = r_0 A^{1/3} n^{1/3}$, $R_i = r_0 A_i^{1/3}$ and Θ is the step function. The volume available to the N fragments writes:

$$\Omega_{eff}(N) = \prod_{l=1}^N \int_{\Omega} d\mathbf{r}_l \theta_l^r \prod_{i<j}^N \theta_{ij} . \quad (2.1)$$

From now on we will explicitly deal with the ratio between Ω_{eff} and Ω^N , χ . As mentioned earlier, one can evaluate this quantity by means of a simple Monte Carlo technique consisting of placing randomly each of the N fragments in the considered freeze-out recipient. The event is considered successful if no two fragments are overlapping each other and no fragment is intersecting the recipient walls. Supposing that one obtains N_s successful events from N_t attempts, one can estimate χ according to:

$$\chi = \frac{N_s}{N_t}. \quad (2.2)$$

Since the relative statistical error in evaluating (2.2) is of the order of $1/\sqrt{N_s}$, it results that for accurate evaluations of small χ values (which is the case of large N) one needs a very large number of generated events (N_t) which makes the method unpracticable. For this reason, a Metropolis-type simulating procedure for calculating χ is further proposed.

Using (2.1) one obtains

$$\frac{\Omega_{eff}(N)}{\Omega_{eff}(N-1)} = \Omega g_N f_N, \quad (2.3)$$

and, by recurrence,

$$\chi = \prod_{k=1}^N g_k f_k, \quad (2.4)$$

where $g_k = \int_{\Omega} d\mathbf{r}_k \theta_k^r / \Omega = [(R - R_k)/R]^3$ and

$$f_k = \frac{\int_{\Omega} d\mathbf{r}_1 \theta_1^r \int_{\Omega} d\mathbf{r}_2 \theta_2^r \theta_{12} \dots \int_{\Omega} d\mathbf{r}_k \theta_k^r \theta_{1k} \dots \theta_{k-1 k}}{\int_{\Omega} d\mathbf{r}_1 \theta_1^r \int_{\Omega} d\mathbf{r}_2 \theta_2^r \theta_{12} \dots \int_{\Omega} d\mathbf{r}_{k-1} \theta_{k-1}^r \theta_{1 k-1} \dots \theta_{k-2 k-1} \int_{\Omega} d\mathbf{r}_k \theta_k^r}. \quad (2.5)$$

The last expression can be regarded from the point of view of a statistical ensemble corresponding to a system consisting of the first k ($\in \{2, \dots, N\}$ - we don't need to consider $k = 1$ since $f_1 = 1$) fragments from the considered partition, composed of configurations $C : \{\mathbf{r}_i, i = 1, \dots, k\}$ and subject to the constraints $\prod_{i < j}^{k-1} \theta_{ij} \prod_{i=1}^k \theta_i^r$. This way, equation (2.5) can be re-written as follows:

$$f_k = \frac{\sum_C \theta_{1k} \dots \theta_{k-1 k}}{\sum_C 1} = \langle \theta_{1k} \dots \theta_{k-1 k} \rangle_k, \quad (2.6)$$

where $\langle \cdot \rangle_k$ has the meaning of average value over the states of the above mentioned ensemble. Therefore, it is sufficient that one knows the values of f_k for $k = 2, \dots, N$ in order to obtain χ . These values can be evaluated using (2.6) within a Metropolis-type simulation which is further described.

For evaluating f_k one just has to generate a Markovian walk in the configuration space of the k fragment system according to the detailed balance principle:

$$\Delta C W_C P(C \rightarrow C') = \Delta C' W_{C'} P(C \leftarrow C'), \quad (2.7)$$

where ΔC and $\Delta C'$ are the elementary volumes of the configurations C and C' , W_C and $W_{C'}$ their statistical weights (here equal to unity) and $P(C \rightarrow C')$ and $P(C \leftarrow C')$ are the probabilities of passing from C to C' and respectively of making the reverse move.

The random walk is generated as follows. Suppose that the current state of the system is C . One chooses at random one of the k fragments, indexed by i and positioned at \mathbf{r}_i . One randomly re-positions this fragment into a spherical volume having the same center as the freeze-out recipient and the radius $R - R_i$ (this ensures the non-overlapping between the fragment and the recipient wall). We denote the chosen position of the fragment i with \mathbf{r}'_i . At this point one has to check whether the constraints of the system are satisfied. So, if $i \neq k$ and the fragment in its new position is overlapping at least one of the remaining fragments indexed from 1 to $k - 1$, the move is aborted and configuration C is reconsidered. Otherwise, the configuration C' is correct and is considered as a new configuration of the system. The probability of this move is:

$$P(C \rightarrow C') = \frac{d\mathbf{r}'_i}{4\pi(R - R_i)^3/3}. \quad (2.8)$$

The probability of the reverse move, similarly generated, writes:

$$P(C \leftarrow C') = \frac{d\mathbf{r}_i}{4\pi(R - R_i)^3/3}. \quad (2.9)$$

Taking into account that $\Delta C = d\mathbf{r}_i \prod_{j \neq i}^k d\mathbf{r}_j$, $\Delta C' = d\mathbf{r}'_i \prod_{j \neq i}^k d\mathbf{r}_j$ and that $W_C = W_{C'}$, one may easily see that the detailed balance equation, (2.7) is satisfied. At this point the exploration of the configuration space is completely described. For calculating f_k one just has to apply formula (2.6), i.e. to determine the average value of the observable $\prod_{i=1}^{k-1} \theta_{ik}$ over the states selected by the simulation. For a number of N_s *successful* (for which $\prod_{i=1}^{k-1} \theta_{ik} = 1$) accepted events the relative statistical error in estimating f_k is of the order of $1/\sqrt{N_s}$.

Provided that f_k was evaluated for each $k \in \{2, \dots, N\}$ using the above described simulation, χ can be obtained using (2.4). Assuming that each simulation (corresponding to a given k) is performed using N_s successful accepted events, then the relative statistical error in evaluating χ is of the order of $\sqrt{N/N_s}$.

III. OVERALL RESULTS

In order to verify the accuracy of the proposed simulation we present in Fig. 1 a comparison between $\chi(N)$ calculated with the present simulation and that calculated with the direct Monte Carlo procedure briefly described at the beginning of Section I in the case of $A = 100$, $\Omega = 10 \Omega_0$ (i.e. $n = 10$). For this evaluation we considered N in a relatively small range (2 to 17) because for larger N the direct Monte Carlo calculation would require unreasonable computing time. The fragment partitions corresponding to each N are randomly¹

¹Starting from the source nucleus one randomly splits it in two fragments. Then, one randomly chooses one of the resulted fragments and splits it randomly in two fragments. The process is repeated until N fragments are obtained. This method has the advantage of generating partitions with χ taking values from a wide range for a given N . The dispersions of χ obtained using this generating procedure are even larger than those obtained using partitions realistically generated (i.e. by means of a microcanonical multifragmentation model). This can be easily checked by comparing the dispersions of χ (corresponding to $n = 6$) from Fig. 2 with those from Fig. 8.

selected. This calculation was performed for $N_s = 10^4$ successful events implying that the relative errors are smaller than the dimension of the points. The same N_s is used in all the calculations presented in this paper. One can observe that the results of the two calculations are practically identical.

For having a preliminary overall look on the simulation results, we calculate χ for $A = 200$ and $n = 4, 6, 8, 10, 14, 20$ for N ranging from 2 to 30 with a step of 1. For each considered N , 5 simulations are performed corresponding to randomly chosen partitions. This allows to evaluate the variation of χ for partitions having the same N . The results are presented in Fig. 2. One can observe that while globally $\log_{10} \chi$ has a linear behavior, variations of orders of magnitude, strongly increasing with decreasing n can be observed for χ corresponding to different partitions with the same N .

In order to test to what extent the assumption of nonoverlapping between the fragments and the recipients' wall is contributing to the above mentioned result, we run the same simulation without imposing this boundary any longer (i.e. the constraints are $\prod_{i < j}^N \theta_{ij}$). Calculations of χ are performed for $A = 200$ and $n = 3, 4, 6, 8, 10, 14, 20$ for N ranging from 2 to 30 with a step of 1 and 10 randomly chosen partitions per each N value (see 3). Due to this relaxation, the effective free volume is now larger so the dependencies $\log_{10} \chi(N)$ are less abrupt than in the previous case (see Fig. 2) and their dispersion is smaller. Nevertheless, variations of χ of orders of magnitude corresponding to partition with the same N , strongly increasing with decreasing n , can be identified here as well.

This suggests that parametrizations of χ solely dependent on N are quite inadequate for cases with relatively small values of n - typically used in multifragmentation studies. One therefore needs a parametrization of χ valid over a large range of N , independent of A and taking into account the above-evidenced strong variation of χ when N and n are kept constant. This problem is addressed in the next section.

From now on we will concentrate exclusively on the initial boundary assumption (i.e. nonoverlapping between the fragments and the recipient walls).

IV. PARAMETRIZATION

The aim of this section is to provide an accurate parametrization of χ which takes into account the strong variation of this quantity for partitions with the same number of fragments. Replacing the expression of χ (corresponding to the case in which the fragments are allowed to intersect the recipients' walls):

$$\chi = \prod_{l=1}^N \frac{\int_{\Omega} d\mathbf{r}_l \prod_{i < j}^N \theta_{ij}}{\int_{\Omega} d\mathbf{r}_l} \quad (4.1)$$

by the following "factorization":

$$\chi' = \prod_{i < j}^N \frac{\int_{\Omega} d\mathbf{r}_i \int_{\Omega} d\mathbf{r}_j \theta_{ij}}{\int_{\Omega} d\mathbf{r}_i \int_{\Omega} d\mathbf{r}_j} = \prod_{i < j}^N \frac{\int_{\Omega} d\mathbf{r}_i \int_{\Omega} d\mathbf{r}_j (1 - \bar{\theta}_{ij})}{\int_{\Omega} d\mathbf{r}_i \int_{\Omega} d\mathbf{r}_j} = \prod_{i < j}^N (1 - P_{ij}), \quad (4.2)$$

where $\bar{\theta}_{ij} = 1 - \theta_{ij}$ and $P_{ij} = (\int_{\Omega} d\mathbf{r}_i \int_{\Omega} d\mathbf{r}_j \bar{\theta}_{ij}) / (\int_{\Omega} d\mathbf{r}_i \int_{\Omega} d\mathbf{r}_j)$, one easily recognizes the two-body approximation due to Cole, Heuer and Charvet [8]. Note that here P_{ij} has the

meaning of probability of overlapping between the particles i and j when they are randomly generated into the volume Ω . A more convenient form for (4.2) is:

$$\ln \chi' = \sum_{i < j}^N \ln (1 - P_{ij}) \quad (4.3)$$

which for small values of P_{ij} can be approximated by:

$$\ln \chi_v = - \sum_{i < j}^N P_{ij}. \quad (4.4)$$

The last expression is the so called virial approximation proposed by Randrup, Robinson and Sneppen [5]. While the exact expression of the two particle overlapping probability, P_{ij} , was deduced in [8], we prefer the simplest approach [5]:

$$P_{ij} = \left(\frac{R_i + R_j}{R} \right)^3. \quad (4.5)$$

Obviously, since it neglects the higher order interactions between fragments and allows intersections of the fragments with the recipients' walls, this approximation overestimates χ . Nevertheless, apart from other approaches (see e.g. [6,7] used in chemical physics calculations) the “virial” approximation has the advantage that it is very simple and that it explicitly accounts for the volume of the freeze-out recipient (thus being appropriate for multifragmentation studies). As we shall further see, this approach provides the basis for a very accurate parametrization of the free volume.

In order to estimate the difference between the virial evaluations (χ_v) and the exact χ , evaluated by means of the method proposed in Section II, we represented in Fig. 4 the ratio $\ln \chi / \ln \chi_v$ calculated over a large range of N (sufficient for the systems currently considered in multifragmentation studies), for four values of n : 4, 6, 8 and 10. For each considered N a fragment partition was generated as in Section III. The considered source is $A = 300$. Though the fragment partitions are generated as to induce an important dispersion in χ (see Fig. 2), $\ln \chi / \ln \chi_v$ has a smooth behavior. In order to have an estimate of the fluctuations of the $\ln \chi / \ln \chi_v(N)$ dependency, we evaluate this quantity for $n = 6$, $A = 300$, N ranging from 2 to 24 and 10 randomly chosen partitions for each value of N . (see Fig. 5). Though the fluctuations are increasing with decreasing N they lay in reasonable limits and are practically negligible for $N > 10$.

Therefore, one can obtain accurate fits of $\ln \chi / \ln \chi_v(N)$ with appropriate functions. As shown in Fig. 4, the function:

$$f(N) = \frac{a N + b}{N^c + d N^e} \quad (4.6)$$

provides a good fit for $\ln \chi / \ln \chi_v$ versus N , for all considered n . The corresponding parameters are listed in Table I. Knowing $f(N)$ for a given n , the real $\ln \chi$ can be expressed as:

$$\ln \chi = \ln \chi_v f(N), \quad (4.7)$$

with $\ln \chi_v$ given by (4.4). In order to test this parametrization, in Fig. 6 are represented versus N χ calculated using the method from Section II and χ evaluated by means of (4.7) for $n=4, 6, 8, 10$. The fragment partitions were considered as in the previous paragraph. The range of N is considered only up to $N = 100$ just for the clarity of the plot. As one can see, the agreement is remarkably good. It thus appears that the present parametrization has the ability of describing accurately the strong variations of χ for different partitions having the same N . Moreover, since for a given partition χ only depends on the fragment *relative* size distribution, it results that this parametrization is independent on A . Some applications and tests of this parametrization are presented in the next section.

V. APPLICATION TO A MICROCANONICAL MULTIFRAGMENTATION MODEL

In this section some supplemental tests for the accuracy of the parametrization proposed in Section IV performed with the sharp microcanonical multifragmentation model from Ref. [10,11] are presented. This model sharply conserves the number of nucleons (A) the number of protons (Z), the total energy (E) and the total momentum (\mathbf{P}) and assumes equal probability of appearance of all possible configurations $C_1 : \{A_i, Z_i, \mathbf{r}_i, \epsilon_i, \mathbf{p}_i, i = 1, \dots, N\}$, where the parameters under the brackets are respectively the mass number, the atomic number, the position, the excitation energy and the momentum of each of the N fragments composing the respective configuration. Integrating the expression of the total number of states of the system over the fragment momenta one reduces the configuration space and works into a new one, composed of configurations $C : \{A_i, Z_i, \mathbf{r}_i, \epsilon_i, i = 1, \dots, N\}$ having statistical weights of the form:

$$W_C = \frac{1}{N!} \prod_{i=1}^N \left[\frac{\rho_i(\epsilon_i)}{h^3} (mA_i)^{3/2} \right] \frac{2\pi}{\Gamma(\frac{3}{2}(N-1))} \frac{(2\pi K)^{\frac{3}{2}N - \frac{5}{2}}}{(mA)^{\frac{3}{2}}}, \quad (5.1)$$

where ρ_i is the level density of the fragment i , m is the mass of a nucleon, $\Gamma()$ is the hyper-geometric function and K is the kinetic energy of the given partition and can be expressed as: $K = E + \sum_i B_i - \sum_i \epsilon_i - \sum_{i<j} V_{ij}$. Here B_i is the binding energy of the fragment i and V_{ij} is the two-body Coulomb interaction energy. The weight of a configuration $C' : \{A_i, Z_i, \epsilon_i, i = 1, \dots, N\}$ corresponding to a new space where the fragment positions are now missing, can be written as:

$$W_{C'} = \prod_{l=1}^N \int_{\Omega} d\mathbf{r}_l W_C \theta_l^r \prod_{i<j}^N \theta_{ij}, \quad (5.2)$$

where Ω , θ_l^r and θ_{ij} have the same meaning as in the previous sections. Now, it can be observed that if one replaces the multi-body Coulomb interaction depending on the fragment positions (entering in K and therefore in W_C) by a single particle mean-field approach, W_C no longer depends on \mathbf{r}_i and (5.2) can be rewritten as:

$$W_{C'} = \Omega^N \chi W_C. \quad (5.3)$$

As one can see, in this case χ manifests as a factor entering the statistical weight of a given configuration, C' . The average value of any system observable X is evaluable in this

new ensemble by: $\langle X \rangle = \sum_{C'} W_{C'} X_{C'} / \sum_{C'} W_{C'}$. For doing this one applies identically the Metropolis simulation proposed in [10,11] except that the positions are no longer generated. The resulted correction factor, α is the same as in Ref. [10,11] except for the factor $\chi(C'_{N+1})/\chi(C'_N)$ appearing now due to the modification of the configuration weights (see equation. (5.3)). For the Coulomb interaction the Wigner-Seitz approach is employed adjusted with a factor as to provide accurate descriptions of the total Coulomb energy even in cases with small N :

$$V_C = V_{WS} g(N), \quad (5.4)$$

with

$$V_{WS} = \frac{3}{5} \frac{Z^2 e^2}{R} - \sum_i \frac{3}{5} \frac{Z_i^2 e^2}{R_i^c}, \quad (5.5)$$

where $R_i^c = R_i n^{1/3}$, V_{WS} is the Wigner-Seitz energy and the factor $g(N) = (1.07675 N + 18.5266)/(N + 14.9439)$ correspond to $n = 6$, which is the case for which the microcanonical calculations are here performed. This factor was evaluated by fitting the ratio between the average Coulomb energy (evaluated by uniformly generating the fragments from a given partition into the spherical recipient such as they are not overlapping each other - this is performed by simple Metropolis moves) and the corresponding V_{WS} versus N . It is worth mentioning that, included in the microcanonical model, this parametrization insures practically identical results with those obtained with the unmodified version of the model.

For testing the accuracy of the free-volume parametrization two types of simulations are performed via the microcanonical multifragmentation model. In the first simulation we just replace the multi-body Coulomb interaction energy with the Wigner-Seitz approach exposed above. Except this detail, the simulation is identical with that from Refs. [10,11] and therefore the fragment positions are explicitly generated at each step, the forbidden configurations (in which fragments are overlapping) being automatically rejected. The second simulation is that formulated in the previous paragraph and includes both the Wigner-Seitz parametrization and the free-volume parametrization. In principle, a correct parametrization of χ should provide closely identical results for any system observable. Here we choose to compare the mass distributions calculated within the two simulations for the source nucleus (70, 32) and the excitation energies $E_{ex}=2$ MeV/nucleon and $E_{ex}=6$ MeV/nucleon. These are represented in Fig. 6. As one can see, the agreement is very good for both cases fact which supports the present parametrization.

An interesting question is to what extent a free-volume parametrization only dependent on N is appropriate for nuclear multifragmentation studies. For answering this question one needs to obtain for each of the above considered cases a parametrization of χ only dependent on N . To this aim, within the first of the two simulations mentioned in the previous paragraph, for each situation [(70, 32), $E_{ex}=2, 6$ MeV/nucleon] we select at random different fragment partitions, corresponding to each N appearing in the simulation, for which we calculate χ . These are represented in Fig. 7. Since the obtained dependence is rather linear in logarithmic scale we fit these distributions by means of linear functions (see Fig. 7). We then employ the obtained parametrizations $\chi(N)$ in the multifragmentation model and we perform the second type of simulation described in the previous paragraph. The results are represented in Fig. 7 by dashed-dotted lines. As one can observe, the

difference between the mass distributions obtained with this last simulation and the mass distribution corresponding to the first simulation (mentioned in the previous paragraph) are quite significant. This confirms the fact that the dispersion in χ for different partitions having the same N which was illustrated in Figs. 2, 8 produces indeed important deviations of the model results from the real values and, therefore, a parametrization of χ solely dependent on N appears to be inadequate. This result is important since it is well known that most of the existent multifragmentation models employ parametrizations of χ only dependent of N .

Finally, a comparison between $\chi(N)$ corresponding to the partitions considered in the previous paragraph (for the source (70, 32) and $E_{ex}=2, 6$ MeV/nucleon) and the SMM parametrization [1] is performed. According to the SMM prescription one has: $\chi = \{[1 + d(N^{1/3} - 1)/(r_0 A^{1/3})]^3 - 1\}^N / n^N$ where $d=1.4$ fm. The $\chi(N)$ dependencies calculated as described in the previous paragraph are represented in Fig. 9 together with the SMM one calculated for $n = 3$ - the usual SMM assumption (since in the SMM model the free volume parametrization has no explicit dependence on n we prefer to use its standard freeze-out assumption, $n = 3$). Analyzing Fig. 9 one can observe that the SMM $n = 3$ curve is flatter than our calculations performed for the $n = 6$ case. Taking into account that the $\ln \chi(N)$ slope is increasing with decreasing n (see Fig. 2), it follows that the differences between the SMM curve and the exact results corresponding to $n = 3$ are even larger than those observed in Fig. 7 between the exact calculations with $n = 6$ and the SMM $n = 3$ curve.

VI. CONCLUSIONS

In summary, a Metropolis-type procedure was designed in order to describe the volume available to N spherical fragments positioned into a spherical recipient. Apart from the direct Monte Carlo technique, this method allows one (for the first time) to make χ evaluations even for large number of fragments. Calculations of χ for randomly chosen partitions corresponding to various n and N values are evidencing that while, for a given n , χ has a more or less global linear dependence of N in logarithmic scale, variations of orders of magnitude may be identified for χ calculated for different partitions corresponding to the same n and N . This suggests that parametrizations of χ only dependent on N may be inadequate for multifragmentation studies. For this reason a parametrization based on virial approximation [5] adjusted with a calibration function as to fit the exact χ values is proposed further-on. The obtained parametrization describes the χ variations corresponding to different partitions having the same N remarkably well. Calibration parameters have been evaluated for four values of the volume of the recipient, corresponding to $n = 4, 6, 8, 10$. The parametrization is further tested with the microcanonical multifragmentation model from Ref. [10,11]. For doing this, the simulation is run in two forms: first with the inclusion of the Wigner-Seitz approach for the Coulomb interaction but maintaining the fragment positioning into the freeze-out volume and the hard core repulsion and then with including both the Wigner-Seitz approach and the free-volume parametrization obtained in Section IV. Mass distributions obtained with these two types of simulation are compared in two input situations. A very good agreement is to be noticed which supports once again the parametrization obtained in Section IV. Finally a study is made concerning the extent to which a parametrization of χ only dependent on N is appropriate for multifragmentation studies. To this aim, the second simulation was run again this time using a parametrization

of χ only dependent on N . In this last case, important deviations between the mass yields obtained with the first simulation and those obtained with the second one are to be noticed. This suggests parametrizations of χ only dependent on N may induce important deviations of the models' results from the real ones. Comparisons between the evaluated $\chi(N)$ dependencies and the corresponding SMM parametrization show important discrepancies.

Presently, there is a strong debate concerning the role of the freeze-out volume in determining the behavior of various thermodynamical quantities (such as the nuclear caloric curve). It was shown that the inclusion of a free volume parametrization in a statistical multifragmentation model is crucial for a good theoretical description of various experimental isotopic caloric curves [12]. The value of the freeze-out volume was proven to influence the shape of the caloric curve and even the order of a possible phase transition: while larger volumes are generating caloric curves with continuously increasing plateau-like regions [11] (reflected in positive peaks in the heat capacity curves), smaller freeze-out volumes seem to encourage the occurrence of back-bendings in the caloric curves, reflected in negative regions of the heat capacity curves [13]. Even the definition of the freeze-out volume is still intensely discussed: should the statistical ensemble be isochore (see e.g. [2]) or should it be isobar (which implies a smooth variation of the freeze-out volume with the excitation energy - as shown in Ref. [14] this option leads to the appearance of back-bendings in the caloric curves) - see [1]. Recently, nonspherical shapes of the freeze-out recipient have been investigated [15] as well. Recent experimental evaluations of the freeze-out volume using two particles velocity correlations predicted values of n in a wide range: 2.5 - 12.5 [16].

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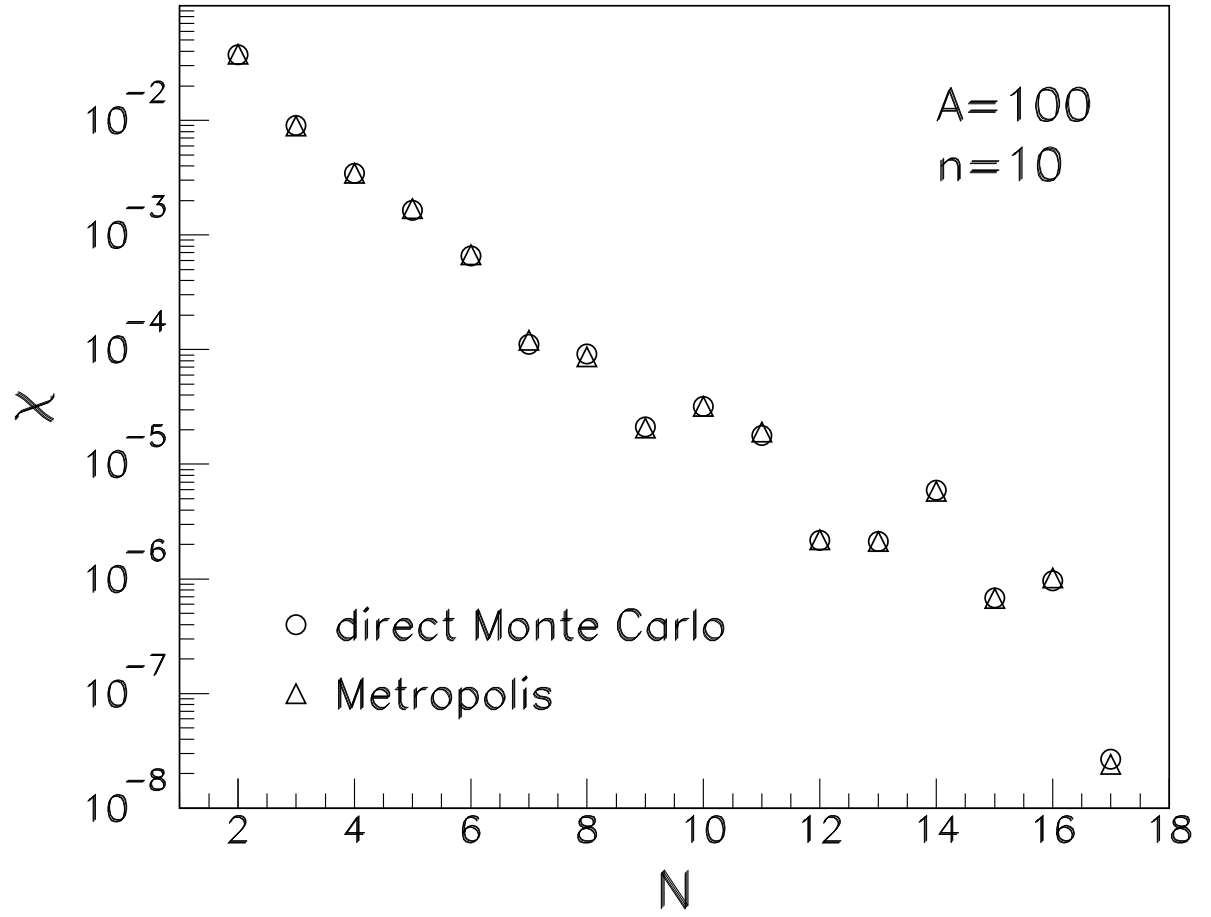


FIG. 1. Comparison between χ values calculated by means of the direct Monte Carlo procedure and those calculated by means of the Metropolis-type simulation for $A = 100$, $n = 10$ and N ranging from 2 to 17. For each N a randomly generated partition was used.

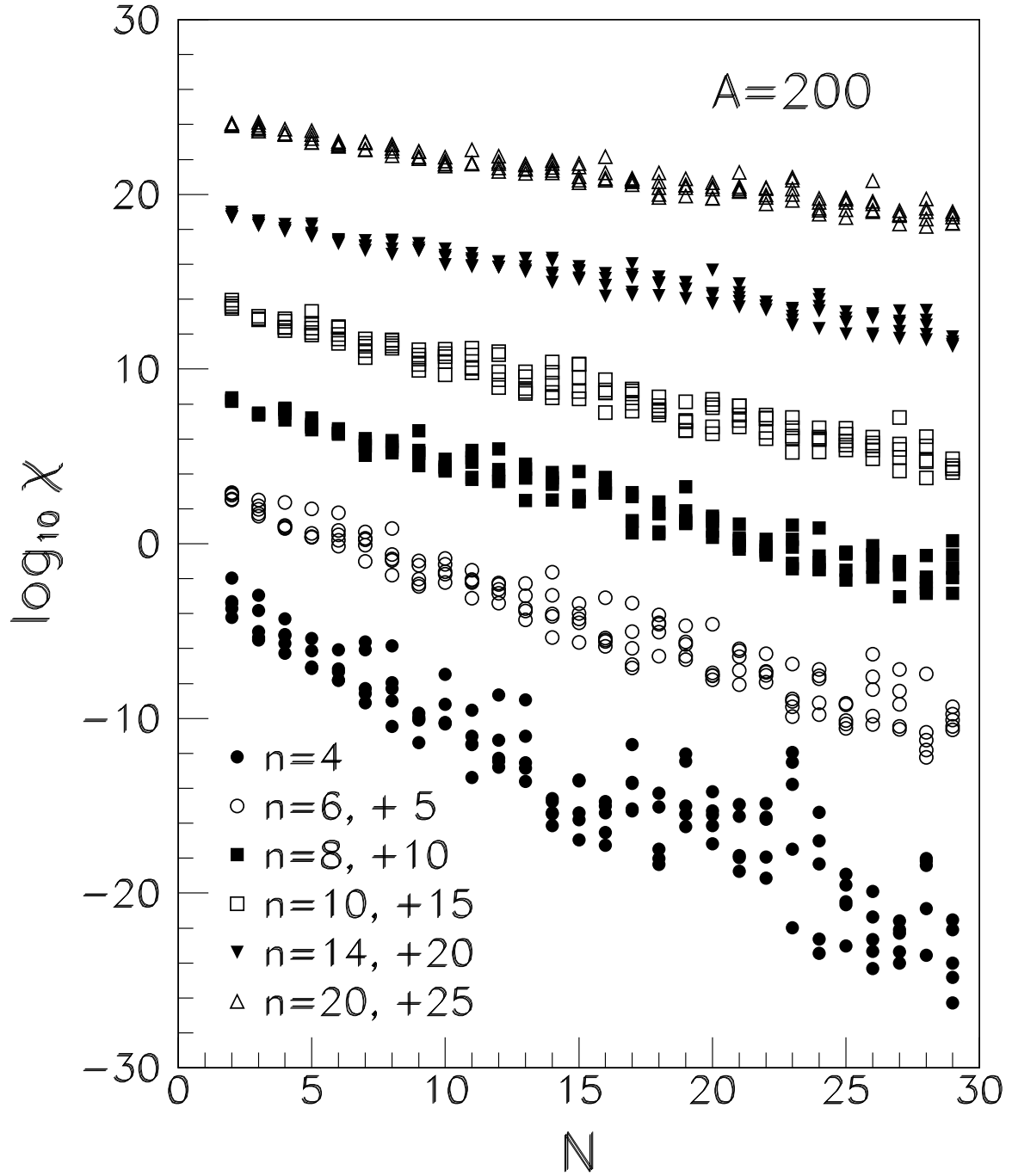


FIG. 2. $\log_{10} \chi$ versus N calculated for six values of n and a source with $A = 200$. For each particular n and N 5 values of $\log_{10} \chi$ are represented, corresponding to randomly chosen partitions. The points corresponding to $n = 6, 8, 10, 14, 20$ are shifted upwards with the quantities specified in the legend in order to avoid overloading.

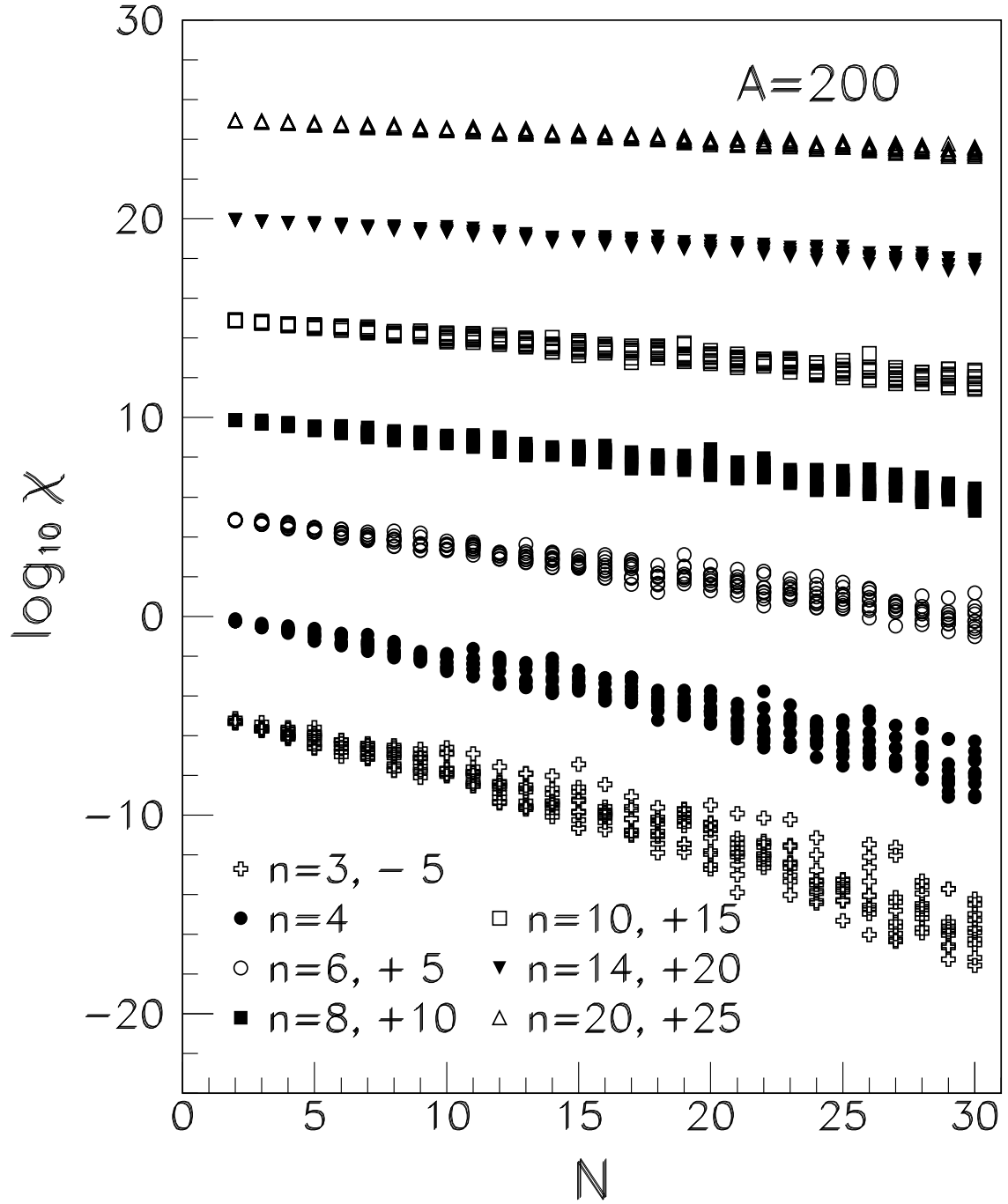


FIG. 3. Same as in Fig. 2 except that the calculations are performed without imposing the constrain of nonintersection between fragments and the recipient wall. Additionally, a calculation corresponding to $n = 3$ is included. For each particular n and N 10 randomly chosen partitions are used in the calculation. Points corresponding to various n are shifted upwards or downwards as shown in the legend in order to avoid overloading.

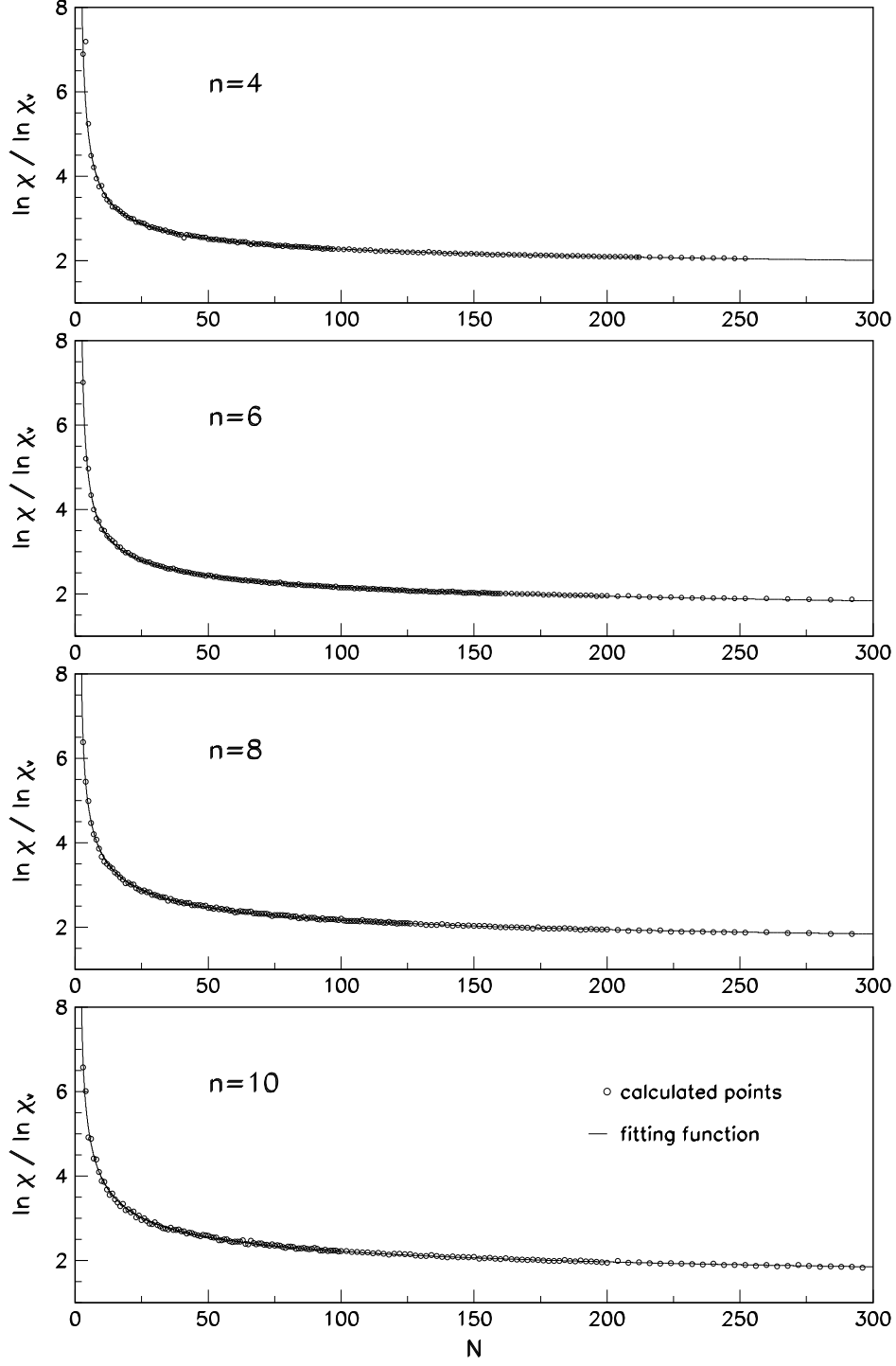


FIG. 4. Ratio between $\ln \chi$ and $\ln \chi_v$ (see the text) versus the number of fragments (N) calculated for $A = 300$ and $n = 4, 6, 8, 10$ fitted with $f(N)$ (see equation (4.6)). The corresponding fitting parameters are listed in Table I.

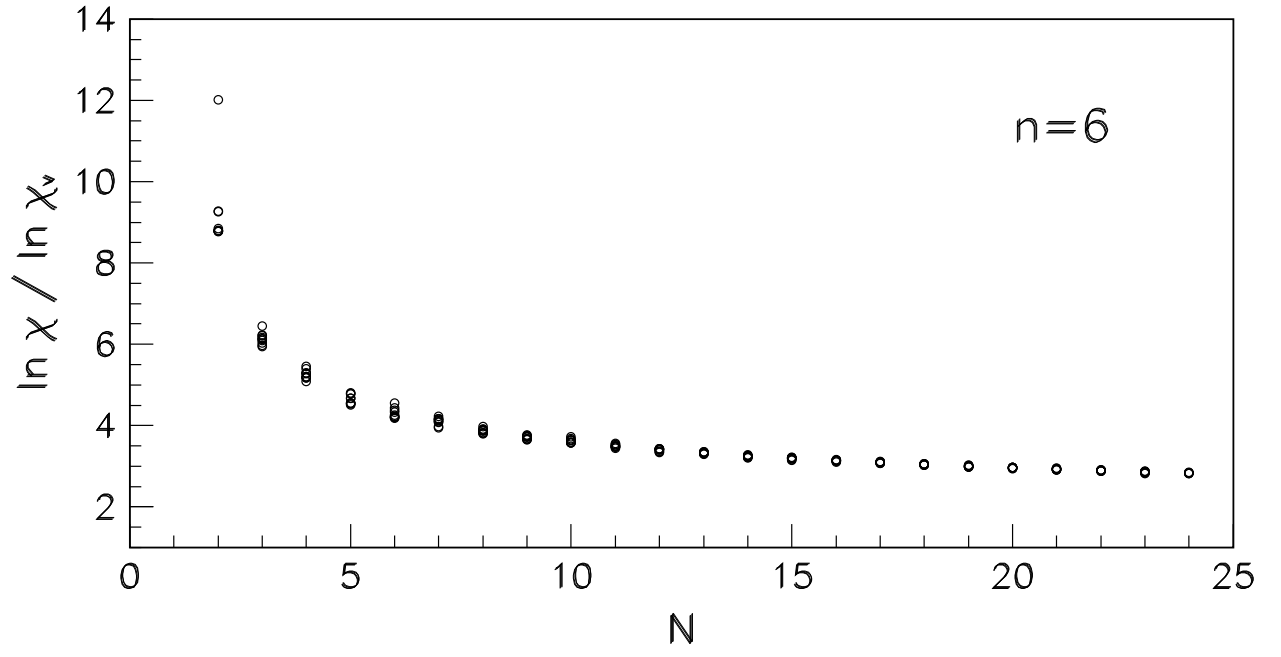


FIG. 5. $\ln \chi / \ln \chi_v(N)$ calculated for $A = 300$, $n = 6$ and 10 randomly chosen fragment partitions for each value of N .

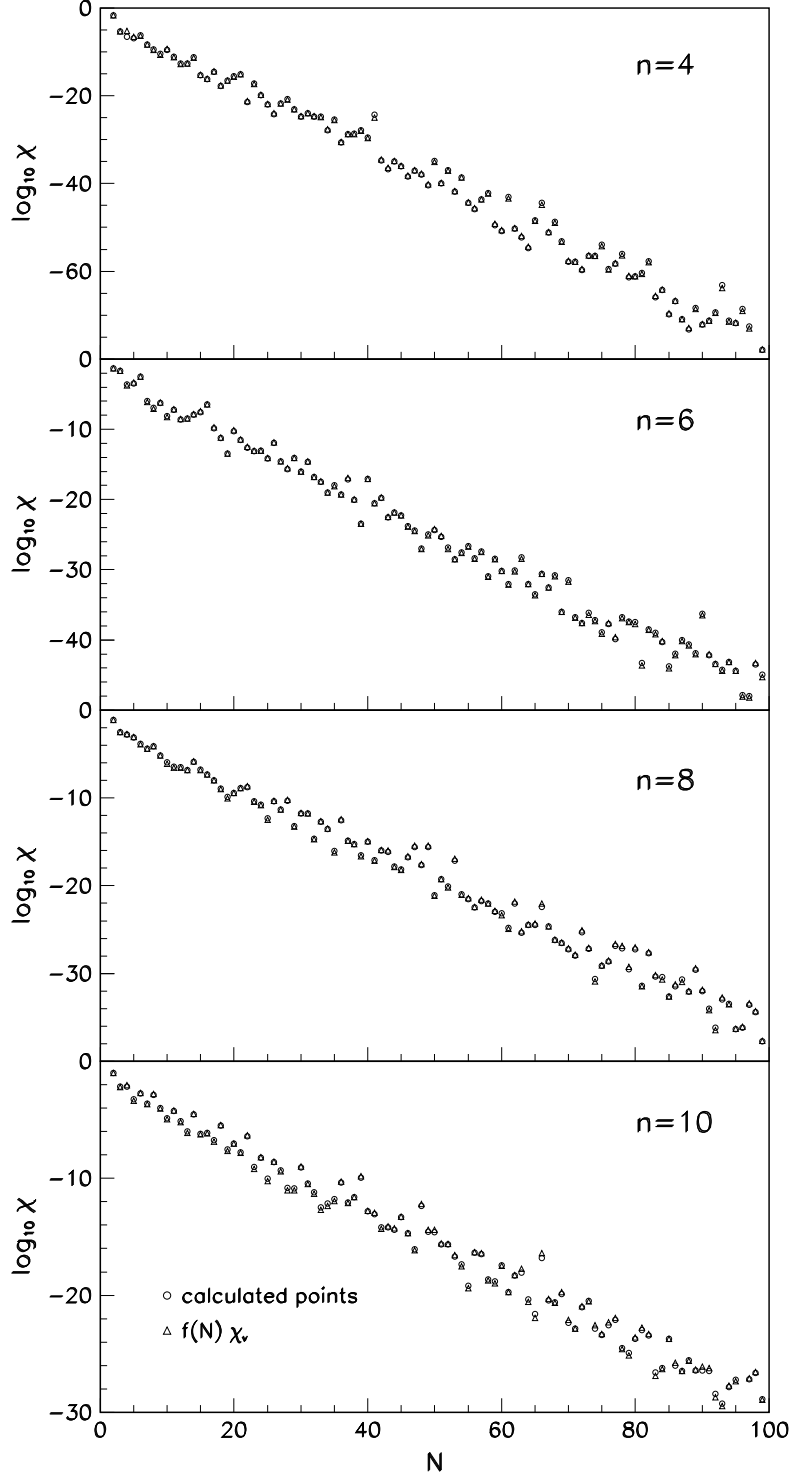


FIG. 6. Calculated $\log_{10} \chi$ versus N corresponding to $A = 300$ and $n = 4, 6, 8, 10$. For each N , χ was calculated for a randomly (see Section III) chosen partition. The circles correspond to calculations using the exact method from Section II and the triangles correspond to the adjusted virial approximation [eq. (4.7)] using the parameters from Table I.

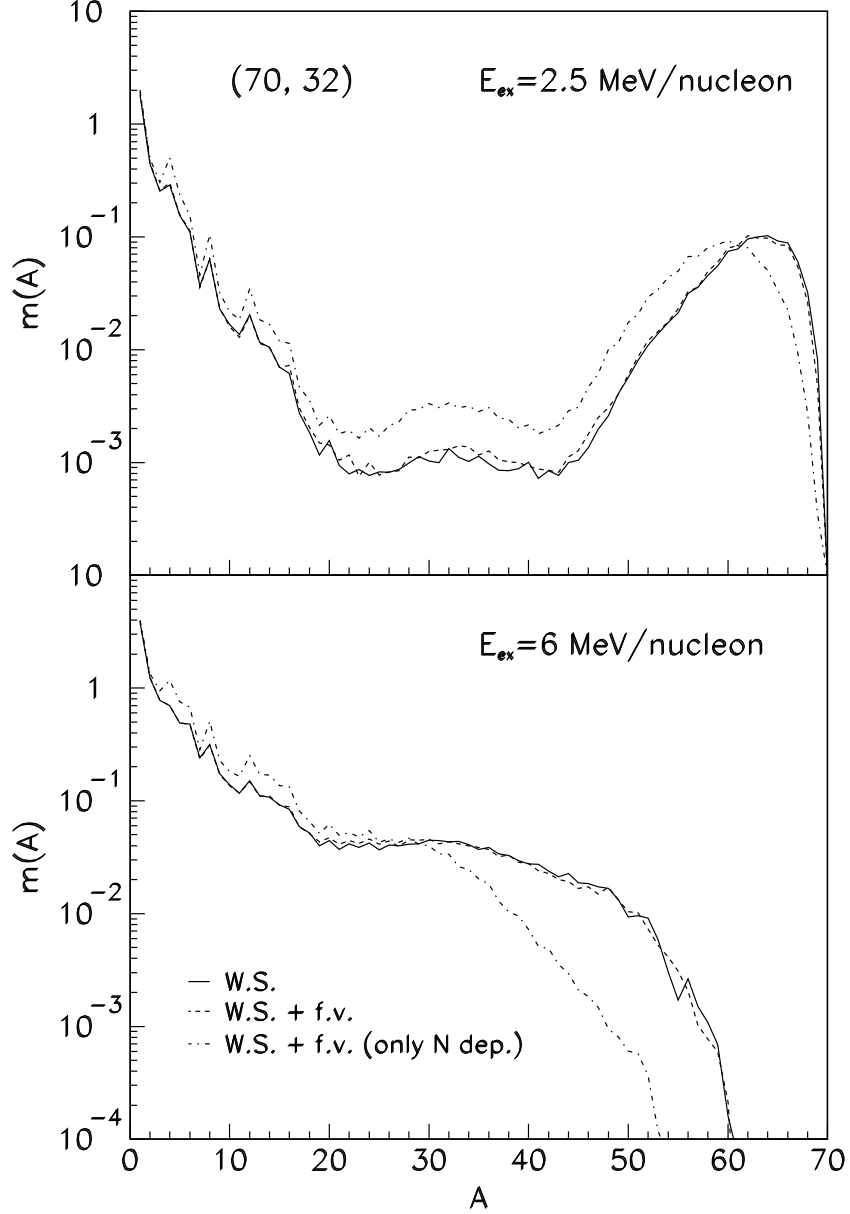


FIG. 7. Fragment mass multiplicities corresponding to the source (70,32) and the excitation energies: 2.5 and 6 MeV/nucleon calculated using the microcanonical multifragmentation model. The continuous lines are calculated using the adjusted Wigner-Seitz (W.S.) approach (see the text) but keeping the fragment positioning into the freeze-out volume, the dashed lines are calculated using both the W.S. approach and the free volume (f.v.) parametrization (4.7) and the dashed-dotted lines correspond to the W.S. approach and a f.v. parametrization only dependent on N (see Fig. 6).

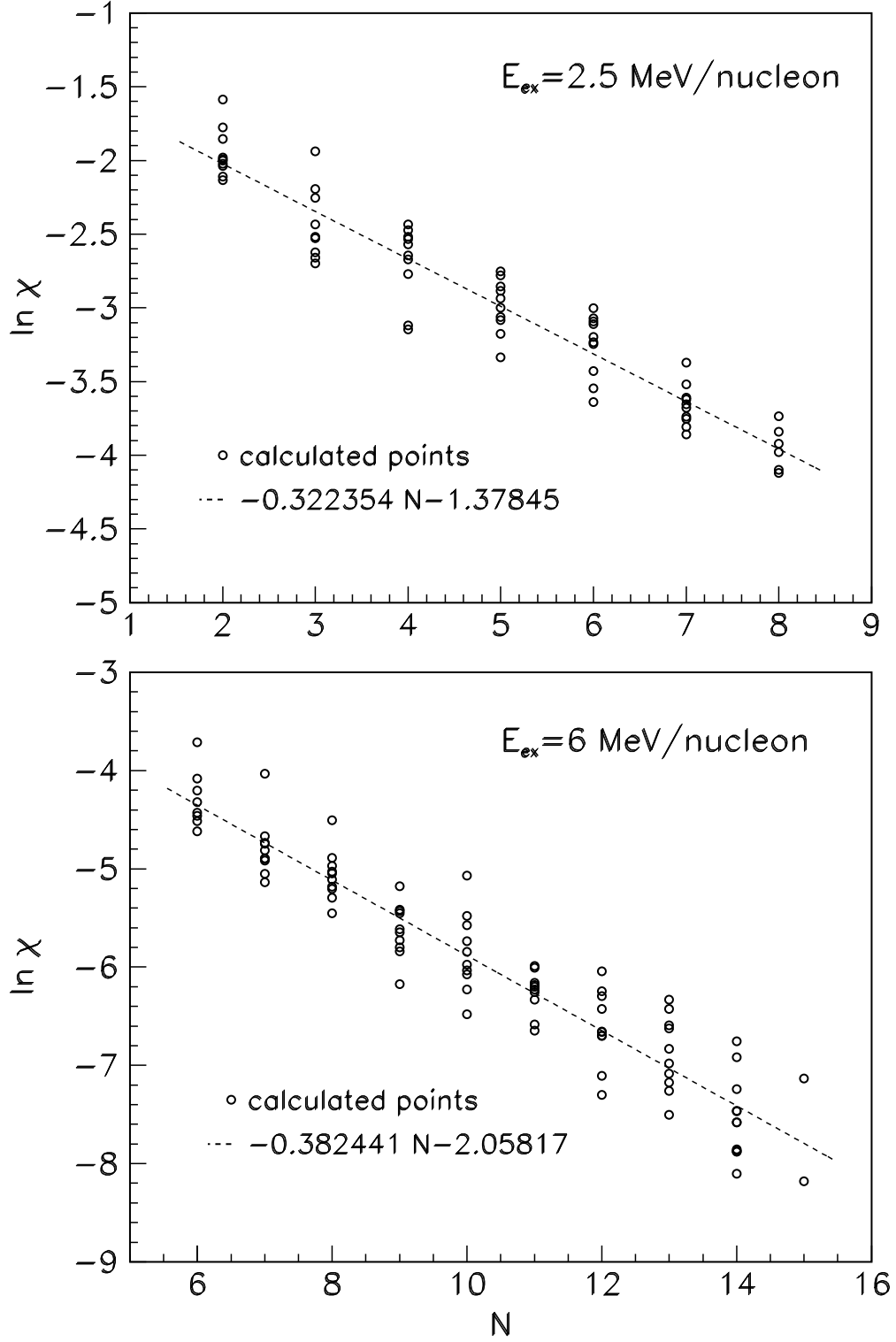


FIG. 8. $\ln \chi$ versus N calculated for the fragment partitions appearing in the fragmentation of the (70,32) source nucleus for the excitation energies 2.5 and 6 MeV/nucleon. Linear fits of $\ln \chi(N)$ are represented by dashed lines. The partitions corresponding to each N are randomly selected from the output of the microcanonical model in which the W.S. approach was used.

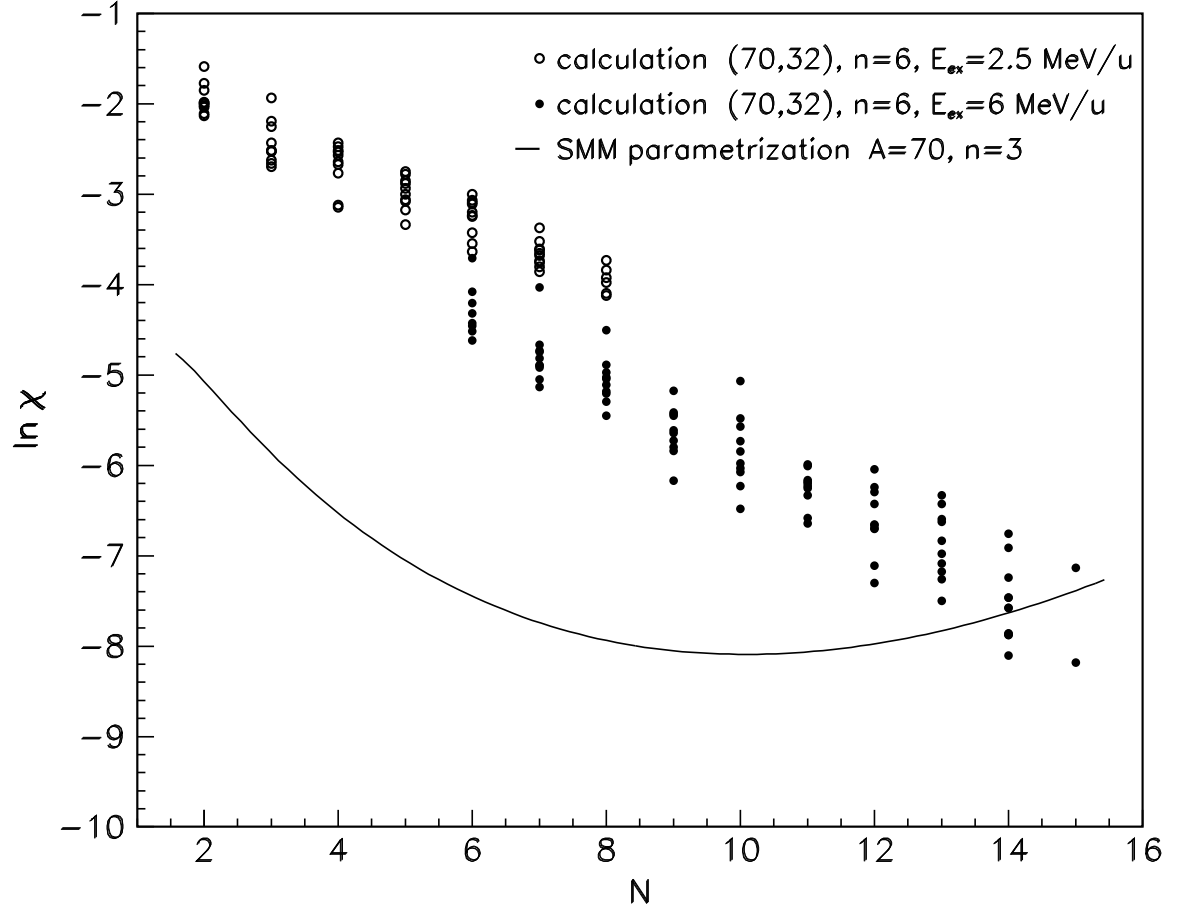


FIG. 9. $\ln \chi(N)$ calculated for the fragment partitions appearing in the fragmentation of the (70,32) source nucleus for the excitation energies 2.5 and 6 MeV/nucleon and $\ln \chi(N)$ corresponding to the SMM free volume parametrization for the case of $A = 70$ and $n = 3$.

n	a	b	c	d	e
4	2.189191	1.096606	1.042162	-0.934725	0.711251
6	3.665597	-0.599464	1.125311	-1.202542	0.432149
8	0.927222	-1.519126	0.999927	-1.085739	0.863371
10	1.117942	-1.976695	1.020913	-1.100722	0.870260

TABLE I. The parameters of the function $f(N)$ [(4.6)] corresponding to four values of n .

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